

1,1,2,3,3,3-Hexafluoro-1-propene
116-15-4 | DTXSID2026949

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.85 | 0.69 | 0.86 | 0.67 | 0.86 | 0.78 |

Model Results

Predicted value: 1.80

Global applicability domain: Inside

Local applicability domain index: 3.68e-01

Confidence level: 7.57e-01

Nearest Neighbors from the Training Set

| | | |
|--|--|--|
| <div>Image not found</div> <div>Hexafluoroacetone</div> <div>Measured: 1.46</div> <div>Predicted: 1.55</div> | <div>Image not found</div> <div>Ethane, hexafluoro-</div> <div>Measured: 2.00</div> <div>Predicted: 1.91</div> | <div>Image not found</div> <div>Ethyl perfluoropropionate</div> <div>Measured: 2.12</div> <div>Predicted: 2.04</div> |
| <div>Image not found</div> <div>1,1,1,3,3,3-Hexafluoro-2-propanol</div> <div>Measured: 1.66</div> <div>Predicted: 1.56</div> | <div>Image not found</div> <div>Isoflurane</div> <div>Measured: 2.06</div> <div>Predicted: 2.08</div> | |